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**NCCS Cluster #2**  
**Series of Brown Bag Presentations**  
**October 2006**

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**NASA Center for Computational Sciences (NCCS)**  
**Computational & Information Sciences and Technology Office (CISTO)**  
**Goddard Space Flight Center**



## Schedule over next few weeks

- **9 October**
  - Final software installations, including PBS
  - Security scans, LDAP integration, etc.
- **16 October**
  - Major power outage in install UPS
  - GPFS metadata configuration and testing
  - System on-line, very early access users
- **23 October**
  - Finalize GPFS
  - Fail over configuration
  - Early access users
- **30 October**
  - Pioneer users
- **6 November**
  - Beginning of acceptance
  - General user access

# Home, nobackup, project file systems

File System	Type	Login	Gateway	Compute
<b>/discover/home/&lt;username&gt;</b> <ul style="list-style-type: none"> <li>• symlinked to /home/&lt;username&gt; (\$HOME)</li> <li>• potentially make this available on explore</li> <li>• quotas with initially small storage space (~500 MB)</li> </ul>	GPFS	Yes	Yes	Yes
<b>/discover/nobackup[1-4]/&lt;username&gt;</b> <ul style="list-style-type: none"> <li>• symlinked to /nobackup/&lt;username&gt; (\$NOBACKUP)</li> <li>• potentially make this available on explore</li> <li>• quotas with initially a large storage space (~100 GB)</li> <li>• not skulded initially (possible GPFS skulking)</li> </ul>	GPFS	Yes	Yes	Yes
<b>/explore/home/&lt;username&gt;</b> <ul style="list-style-type: none"> <li>• NFS mounted from explore</li> </ul>	CXFS NFS	Yes	Yes	<b>No</b>
<b>/explore/nobackup[1-4]/&lt;username&gt;</b> <ul style="list-style-type: none"> <li>• NFS mounted from explore</li> </ul>	CXFS NFS	Yes	Yes	<b>No</b>
<b>/discover/nobackup[1-4]/project/&lt;projectname&gt;</b> <ul style="list-style-type: none"> <li>• project specific directories</li> <li>• space driven by project requirements</li> </ul>	GPFS	Yes	Yes	Yes

# Other file systems

File System	Type	Login	Gateway	Compute
<b>/usr/local</b> <ul style="list-style-type: none"> <li>• /usr/local/otherlibs will be created under here (or whatever you want to call it)</li> </ul>	GPFS	Yes	Yes	Yes
<b>/usr/local/unsupported</b> <ul style="list-style-type: none"> <li>• symlinked to /usr/ulocal</li> </ul>	GPFS	Yes	Yes	Yes
<b>/usr/nlocal</b> <ul style="list-style-type: none"> <li>• node specific local directory (NOT Global)</li> </ul>	Local	Yes	Yes	Yes
<b>/opt</b> <ul style="list-style-type: none"> <li>• MPI libraries stored here</li> <li>• Don't need to worry about this, just load the module</li> <li>• Same on each node (local to each node)</li> </ul>	Local	Yes	Yes	Yes
<b>/g[1-8] and other DMF archive directories</b> <ul style="list-style-type: none"> <li>• symlinked to /archive/&lt;username&gt;</li> </ul> (\$ARCHIVE) - Details TBD	CXFS NFS	Yes	Yes	<b>No</b>



# Currently Available Modules

**borgmg:/ # module avail**

```
----- /usr/share/modules/modulefiles -----  
bgcc/autoconf-2.13      comp/gcc-3.4.6          module-info  
bgcc/gcc-3.2.3          comp/gcc-4.0.3          modules  
bgcc/gcc-3.3.1          comp/gcc-4.1.1          mpi/intel-2.0.1  
bgcc/gcc-3.3.3          comp/intel-8.1.034      mpi/mpich-1.2.7  
bgcc/gcc-3.3.6          comp/intel-8.1.038      mpi/openmpi-1.1  
bgcc/gcc-3.4.3          comp/intel-9.1.038      mpi/scali-5.1.0.1  
bgcc/gcc-3.4.6          comp/intel-9.1.039      mpi/sst-3.3.0.4.1-crc  
bgcc/gcc-4.0.3          comp/intel-9.1.042      mpi/sst-3.3.0.4.1-crc2  
bgcc/gcc-4.1.1          comp/intel-9.1.043      mpi/sst-3.3.0.4.1-crc4  
comp/gcc-3.2.3          comp/pgi-6.1.6          mpi/sst-3.3.0.4.1-crc5  
comp/gcc-3.3.1          dot                      mpi/sst-3.3.0.4.1-crc6  
comp/gcc-3.3.3          lib/mkl-8.1             mpi/sst-3.3.0.8.4  
comp/gcc-3.3.6          lib/mkl-9.0beta        null  
comp/gcc-3.4.3          module-cvs              use.own
```

**Many of which need not be available to the users.**



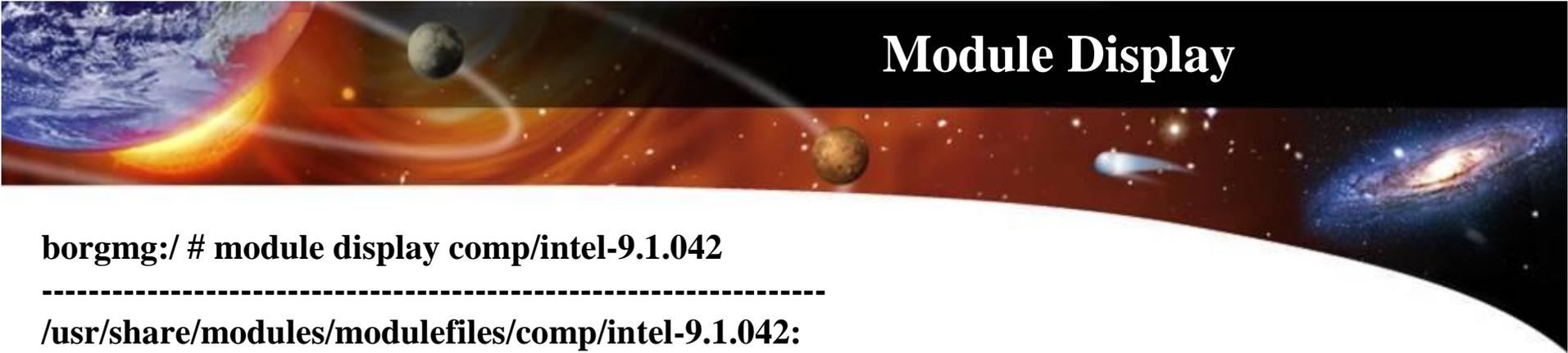
## User Available Modules Something like the following...

**borgmg:/ # module avail**

```
----- /usr/share/modules/modulefiles -----  
comp/gcc-3.4.6  
comp/gcc-4.1.1  
comp/intel-8.1.034  
comp/intel-8.1.038  
comp/intel-9.1.038  
comp/intel-9.1.039  
comp/intel-9.1.042  
comp/intel-9.1.043  
comp/pgi-6.1.6  
lib/mkl-8.1  
lib/mkl-9.0beta  
module-cvs  
module-info  
modules  
mpi/intel-2.0.1  
mpi/mpich-1.2.7  
mpi/openmpi-1.1  
mpi/scali-5.1.0.1  
mpi/sst-3.3.0.8.4  
mpi/sst-3.3.0.8.4-crc  
use.own
```

**Only keep a small number of gcc compiler versions, and a relatively manageable set of Intel compiler versions.**

**As versions are retired, permissions will be changed so they do not show up with a module available listing, but they will still be on the system.**



# Module Display

```
borgmg:/ # module display comp/intel-9.1.042
```

```
-----  
/usr/share/modules/modulefiles/comp/intel-9.1.042:
```

```
conflict      comp  
module-whatis loads the comp/intel-9.1.042 environment  
setenv        INTEL_LICENSE_FILE /usr/local/intel/license  
setenv        COMPILER intel  
setenv        COMPILER_VER 9.1.042  
setenv        CC /usr/local/intel/cce/9.1.042/bin/icc  
setenv        FC /usr/local/intel/fce/9.1.036/bin/ifort  
prepend-path  PATH /usr/local/intel/cce/9.1.042/bin:/usr/local/intel/fce/9.1.036/bin  
prepend-path  LD_LIBRARY_PATH /usr/local/intel/cce/9.1.042/lib:/usr/local/intel/fce/9.1.036/lib  
prepend-path  LIBRARY_PATH /usr/local/intel/cce/9.1.042/lib:/usr/local/intel/fce/9.1.036/lib  
prepend-path  INCLUDE /usr/local/intel/cce/9.1.042/lib:/usr/local/intel/fce/9.1.036/include  
prepend-path  MANPATH /usr/local/intel/cce/9.1.042/man:/usr/local/intel/fce/9.1.036/man  
-----
```

- **Specialized nodes for data movement**
  - Two (2) gateway nodes for the base unit configured with the following
    - Dual socket, dual core Dempsey
    - 8 GB of RAM
    - 10 GbE network interfaces
- **Scheduled via PBS specifically for data movement queues**
  - Single CPU jobs (for data movement only)
  - “datamove” queue will run on these nodes

# Visualization Nodes

- 16 nodes configure into the base unit
  - AMD Opteron dual core 280 processors (2.6 GHz)
  - 8 x 1 GB of PC3200/DDR400 S/R DIMM
  - 250 GB SATA
  - PCI-Express with SilverStorm infiniband 4x HCA (10 Gb)
  - NVidia Quadro FX 4500 PCI-Express
  - 10 GbE network interfaces
- User Environment
  - Same user environment as all other nodes, including additional software like IDL
  - Same file systems and tools
- How will this be used?
  - Future plans call for a potential viz wall
  - Post process, analysis, special processing





## Test and development system

- A small test and development system is being configured to be as identical to the production system as possible
  - Same file system configuration with reduced number of data and metadata servers but with the same failover setup
  - Same management server configuration with failover setup
  - Reduced number of login and gateway systems, but can mimic necessary DNS and other failover scenarios
  - Similar disk subsystems, but not identical
- Is it big enough to test applications?
  - Configuring the system with 10 nodes of Dempsey and will expand to include 10 nodes of Woodcrest later
  - 40 cores of each processor: is that enough?
  - NOT a production system